

# A new broken $U(1)$ -symmetry in extreme type-II superconductors

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A phase transition within the molten phase of the Abrikosov vortex system without disorder in extreme type-II superconductors is found via large-scale Monte-Carlo simulations. It involves breaking a  $U(1)$ -symmetry, and has a zero-field counterpart, unlike vortex lattice melting. Its hallmark is the loss of number-conservation of connected vortex paths threading the entire system *in any direction*, driving the vortex line tension to zero. This tension plays the role of a generalized “stiffness” of the vortex liquid, and serves as a probe of the loss of order at the transition, where a weak specific heat anomaly is found.

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The key role of topological excitations in all phase-transitions, whose proliferation is accompanied by the loss of a generalized “stiffness”, has been emphasized by Anderson<sup>1</sup>. Recent numerical<sup>2–5</sup> and analytical work<sup>6,7</sup> reveals that in extreme type-II superconductors, topological excitations in the form of vortex loops are essential to the physics of the vortex system in low magnetic fields.

It will be shown in this paper that the proliferation of large vortex loops induces a phase transition *within the molten phase* of the Abrikosov vortex system without disorder. The phase-transition thus appears in a region of the phase-diagram where one normally would not expect critical behavior simply based on a study of the *local superconducting order parameter*  $\Psi$  entering Ginzburg-Landau theory. It is, however, a general property of extreme type-II superconductors, distinct from the first order vortex lattice melting transition in that it has a zero-field counterpart, i.e. the transition from a superconductor to a normal metal mediated by a vortex-loop “blowout”<sup>8,9,4,5,7</sup>.

The model for extreme type-II superconductors considered in this paper, is the uniformly frustrated 3 dimensional anisotropic XY (3DXY) model<sup>10</sup>, defined by the Hamiltonian

$$H(\{\theta(\mathbf{r})\}) = - \sum_{\mathbf{r}, \mu=x,y,z} J_{\mu} \cos[\nabla_{\mu}\theta(\mathbf{r}) - A_{\mu}(\mathbf{r})], \quad (1)$$

where  $\theta$  is the local phase angle of the superconducting complex order parameter and  $\nabla$  is a lattice derivative. The coupling energy along the  $\mu$ -axis,  $J_{\mu}$ , is defined by  $J_x = J_y = (\Phi_0^2 d)/(16\pi^3 \lambda_{ab}^2) \equiv J_{\perp}$ , and  $J_z = (\Phi_0^2 \xi_{ab}^2)/(16\pi^3 \lambda_c^2 d)$ , where  $\lambda_{ab}$  and  $\lambda_c$  are the magnetic penetration lengths set up by screening currents in the CuO plane and along the crystal  $c$ -axis, respectively.  $\Phi_0$  is the flux quantum,  $\xi_{ab}$  is the superconducting coherence length within the CuO-planes, and  $d$  is the distance between two CuO-layers in *adjacent unit cells*. We may use the lattice spacing as a measure of  $\xi_{ab}$ . In Eq. 1,  $A_{\mu}$  is related to the non-fluctuating external magnetic vector potential  $\mathbf{A}_{vp}$  by  $A_{\mu}(\mathbf{r}) \equiv 2\pi/\Phi_0 \int_{\mathbf{r}}^{\mathbf{r}+\hat{e}_{\mu}} d\mathbf{r}' \cdot \mathbf{A}_{vp}(\mathbf{r}')$ , where  $\hat{e}_{\mu}$  is the unit vector along the  $\mu$ -axis.

We consider systems of size  $L_x \times L_y \times L_z$ . To perform simulations and finite size scaling of systems with very low filling fractions, we define an “extended” Landau gauge

$$A_x = \frac{2\pi y m_y n m}{L_x L_y}; \quad A_y = \frac{2\pi x n_x m n}{L_x L_y}, \quad (2)$$

where  $n_x, n, m_y, m$  are positive integers satisfying  $n_x n = L_y$ , and  $m_y m = L_x$ . Hence, the filling fraction  $f$  is given by  $f = n m [n_x - m_y]/L_x L_y$ .

In this paper, we consider the filling fractions  $f$  in the range  $1/f \in (20, \dots, 1560)$ . *These filling fractions are so low that spurious pinning to the numerical lattice is eliminated, i.e. any spurious transverse Meissner-effect has vanished, well below all temperatures of interest in this paper*<sup>2–5</sup>. Using  $f = B \xi_{ab}^2/\Phi_0$  and  $\xi_{ab} = 15\text{\AA}$ ,  $1/f = 1560$  corresponds to a uniform induction  $B \sim 0.56T$ . Using  $\lambda_{ab} > a_v$  as a condition for uniform  $B$  and  $\lambda_{ab} = 1500\text{\AA}$ , we find that this assumption is valid for inductions as low as  $0.1T$ , corresponding to a filling fraction of order  $10^{-4}$ . The uniform induction  $B$  is taken along the crystal  $\hat{c}$ -axis. The anisotropy parameter is given by  $\Gamma = \sqrt{J_{\perp}/J_z} = \lambda_c d/\lambda_{ab} \xi_{ab}$ . For each filling fraction, we carry out simulations on three systems with different sizes ( $\sim 40^3, \sim 80^3, \sim 150^3$ ) to study finite-size effects. For the specific heat, we also consider  $360^3$  for  $f = 1/90$ .

In addition to the specific heat  $C$ <sup>4,5</sup>, we calculate three quantities in this paper. The first two are standard, while the third is unusual and probes a subtle  $U(1)$ -symmetry of the system.

*i) Helicity modulus.* To probe the global phase coherence we consider the helicity moduli,  $\Upsilon_{\mu}$ , defined as the second derivative of the free energy with respect to an applied phase twist<sup>11,5</sup>. When  $\Upsilon_{\mu}$  is zero, the resistance along  $\mu$ -direction is finite, and any applied current along  $\mu$ -direction will dissipate energy. Note that  $\Upsilon_{\mu}$  is a global quantity, so even when  $\Upsilon_{\mu} = 0$  the system can still maintain local phase coherence and exhibit diamagnetic fluctuations.  $\Upsilon_z$  will vanish at the temperature  $T_z$ , coinciding with the zero-field superconducting transition  $T_c$  when  $f = 0$ , and will coincide with the melting temper-

ature of the Abrikosov vortex lattice (AVL) when  $f > 0$ .

*ii) Structure factor.* To probe the Abrikosov vortex lattice (AVL) melting, we consider the structure function for  $q_z$  vortex segments<sup>12,2</sup>. A vortex configuration can be obtained from a phase-configuration from the counterclockwise line integral of the gauge-invariant phase-differences around any plaquette of the numerical lattice. It must satisfy the condition for conservation of vorticity,  $\sum_C [\nabla_\nu \theta(\mathbf{r}) - A_\nu(\mathbf{r})] = 2\pi(q_\mu(\mathbf{r}) - f_\mu)$ . Here,  $C$  is the closed path traced out by the links surrounding an elementary plaquette, and  $\nu$  represents the Cartesian components of the links comprising the closed path  $C$ . Furthermore,  $q_\mu(\mathbf{r}) = 0, \pm 1$  represents a vortex segment penetrating the plaquette enclosed by  $C$ . If we monitor the structure function  $S(\mathbf{Q}, k_z = 0)$  of one chosen Bragg peak as a function of temperature, we expect that  $S(\mathbf{Q}, k_z = 0)$  has a discontinuous drop to a very small value at the melting temperature. The structure function will vanish discontinuously at the melting temperature  $T_m(B)$  of the AVL.

*iii) Vortex-path probability  $O_L$ .* We define  $O_L$  as the probability of finding a directed vortex path threading the entire system transverse to the induction  $B$ , *without using the PBC along the field direction*. It is obtained by computing the number  $N_V$  of times we find *at least one* such path threading the system in any direction  $\perp B$  in  $N_P$  different phase-configurations, normalized by  $N_P$ , i.e.  $O_L = N_V/N_P$ . Note that this differs from algorithms employed in previous publications<sup>13,14</sup>.

$O_L = 0$  means that there is no connected path of vortex segments that threads the entire system in the transverse direction, without using PBC along the field direction several times. Now, let  $N_L^\alpha$  ( $\alpha \in [x, y, z]$ ) denote the areal density of connected vortex paths threading the system in any direction, including the direction parallel to the induction. It is clear that in the AVL phase  $O_L = 0$ , and  $N_L^z = B/\Phi_0$ , while  $N_L^x = N_L^y = 0$ . Thus,  $N_L^\alpha$  is a conserved quantity at fixed induction  $B$ . On the other hand,  $O_L = 1$  implies that  $N_L^{x,y} > 0$ , and the *total* number of vortex paths threading the system in any direction scales with system size, but undergoes thermal fluctuations. Therefore,  $N_L^\alpha$  is no longer a conserved quantity. The change in  $O_L$  takes place at the temperature  $T_L(B)$ , which coincides with  $T_c$  when  $f = 0$ .

Number conservation uniquely identifies a  $U(1)$ -symmetry, and hence the low-temperature phase of the *vortex-system* (the dual of the phase-representation of the superconductor) exhibits explicit  $U(1)$ -symmetry, since  $O_L = 0$ . At high temperatures  $O_L = 1$ ,  $N_L^\alpha$  is not conserved, and the  $U(1)$ -symmetry is broken. Under no circumstance can a  $U(1)$ -symmetric phase be analytically continued to a  $U(1)$ -nonsymmetric one. *The change in  $O_L$  from 0 to 1 therefore signals a geometric transition taking place within the vortex-liquid*, indicative of the breakdown of *vortex-line* liquid picture of the molten phase of the Abrikosov vortex lattice.

We first discuss the zero-field simulation results. In

Fig. 1, we plot the specific heat  $C$ , the helicity moduli  $\Upsilon_x, \Upsilon_z$ , and  $O_L$  as functions of temperature for a system with  $Size = 140^3$  and anisotropy  $\Gamma = 7$ .  $C$  has a near-logarithmic singularity at  $k_B T_c/J_\perp = 1.12$ , where also  $\Upsilon_x$  and  $\Upsilon_z$  drop to zero. This second order phase transition is the superconducting-normal state phase transition. Note that both  $\Upsilon_z$  and  $\Upsilon_x$  vanish at  $T_c$ , albeit with different amplitudes due to the anisotropy of the model. Since there is one, and only one, transition in zero field, this is a check that the system sizes used in the simulations are adequate for the given anisotropy<sup>4</sup>.

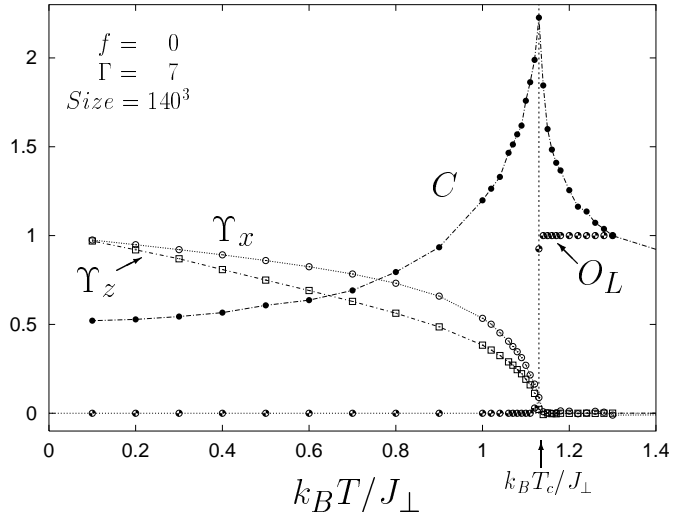


FIG. 1. Specific heat, vortex-path probability  $O_L$ , and helicity moduli along  $x$ -direction ( $\Upsilon_x$ ) and along  $z$ -direction ( $\Upsilon_z$ ) as functions of temperature for the zero field case.  $\Gamma = 7$ , and system size is  $140^3$ . For  $T < T_c$ ,  $O_L = 0$ . For  $T > T_c$  a vortex loop blow out has taken place, i.e.  $O_L = 1$ .

For  $T < T_c$ , it is clear that  $O_L = 0$  and  $N_L^\alpha$  is conserved and equal to zero. If for  $T > T_c$ , we have  $O_L = 1$ , then  $N_L^\alpha > 0$ . This feature of  $O_L$  is precisely what we find in our simulations, see Fig. 1. This means that the system undergoes a  $3DXY$ -transition, with a low-temperature  $U(1)$ -symmetric state and a high-temperature  $U(1)$ -nonsymmetric state. Note that in terms of the ordinary superconducting orderparameter  $\Psi$  in Ginzburg-Landau theory in zero field, the situation is the opposite as far as  $U(1)$ -symmetry and symmetry breaking is concerned: The more familiar phase-representation of the superconductor is related to the vortex-representation via a duality transformation which interchanges low and high temperatures<sup>15</sup>.

Next, we consider finite magnetic fields. In Fig. top panel, we plot the specific heat  $C$ , the structure factor  $S$ ,  $O_L$  and the helicity moduli  $\Upsilon_x$ <sup>16</sup> and  $\Upsilon_z$  as functions of temperature for a system with filling fraction  $f = 1/90$ ,  $Size = 72 \times 80 \times 80$  and  $\Gamma = 7$ . We see from the top panel of Fig. that at  $k_B T_m/J_\perp = 0.49$  the structure factor  $S$  drops discontinuously from 0.2 to 0, indicating a first order AVL melting transition at  $T_m$ . At  $T = T_z$ ,  $\Upsilon_z$  drops discontinuously from 0.55 to 0. We see that in

our simulations  $T_z = T_m$ , indicating that the AVL melts directly into an incoherent vortex liquid. Thus, in the vortex liquid phase there is no global phase coherence in any direction<sup>4,3,5</sup>. This conclusion also holds for the isotropic case  $\Gamma = 1$ <sup>17,18</sup>.

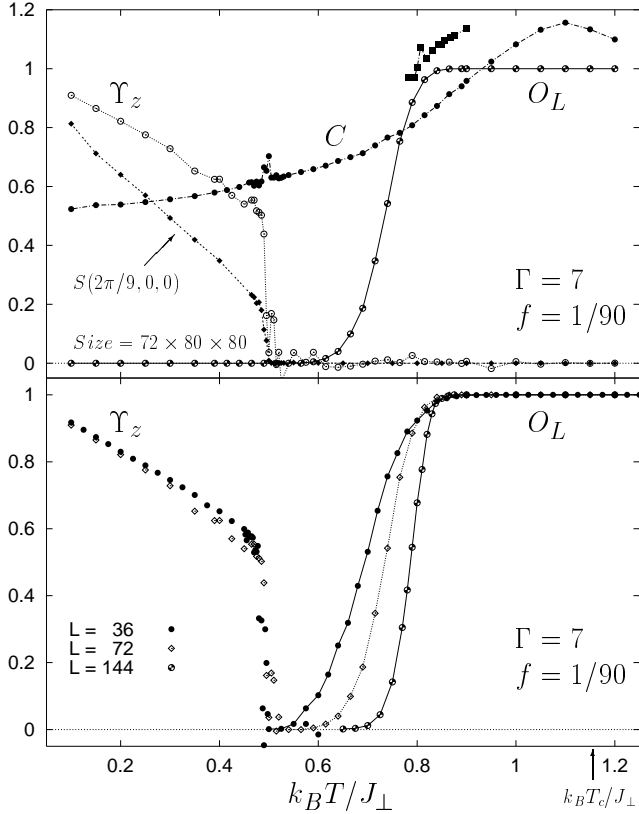


FIG. 1. Top panel: Specific heat  $C$ , structure factor  $S$ , vortex-path probability  $O_L$  and helicity moduli  $\Upsilon_x$ ,  $\Upsilon_z$  as functions of temperature for a system with a filling fraction  $f = 1/90$  and  $\text{Size} = 72 \times 80 \times 80$ . The melting temperature is given by  $k_B T_m / J_\perp = 0.49$ . At  $T_L(B)$ , we also show  $C$  for a system of size  $360^3$ , illustrated by solid squares. The curve is shifted up by the amount  $0.2 k_B$  from the curve for  $72 \times 80 \times 80$ , for clarity. Note the increase in the weak anomaly at  $T_L(B)$ , which is the hallmark of a thermodynamic phase transition.

Bottom panel: Helicity modulus along the field direction  $\Upsilon_z$  and  $O_L$  as functions of temperature for three systems with  $f = 1/90$  and sizes  $36 \times 40 \times 40$ ,  $72 \times 80 \times 80$ ,  $144 \times 160 \times 160$ .

In the top panel of Fig. 1, the specific heat shows a spike precisely at  $T_m$ , indicating a discontinuous jump in the internal energy, and thus proving the existence of a first order phase AVL melting transition with a latent heat at  $T_m$ . We now focus on the temperature range where  $O_L$  changes from 0 to 1. For the filling fraction  $f = 1/90$ ,  $O_L$  rises from 0 to 1, and reaches 1 at  $T = T_L$  well separated from  $T_m$  and the crossover temperature  $T_{Bc2}$ , see top panel of Fig. 1. vortex loop blowout takes place. For in-

creasing system size the width of the transition decreases rapidly, see the lower panel of Fig. 1. Note also how the low-temperature tail of  $O_L$  is suppressed when increasing the system size, while the temperature  $T_L(B)$  where  $O_L$  reaches the value 1 stays almost fixed, moving slightly down with increasing system size. Thus, in the thermodynamic limit, there exists a well defined temperature  $T_L$  where  $O_L$  rises sharply from 0 to 1. This is found for all the filling fractions considered. For  $f = 1/90$ , we have also performed simulations for systems of size  $360^3$ , to bring out the scaling of the additional weak specific heat anomaly at  $T_L(B)$ , see the top panel of Fig. 1. It shows conclusively that  $T_L(B)$  is a thermodynamic phase-transition.

The position of the specific heat anomaly at  $T_L(B)$  for the system of size  $360^3$  appears at a slightly lower temperature than those where  $O_L$  starts to dip down from 1 in smaller systems. This is because the  $O_L$ -curves become sharper as  $L$  increases, and the position of the  $C$ -anomaly is at a position which may be estimated to be the limiting temperature at which  $O_L$  changes abruptly from 0 to 1. Note that in the specific heat, the anomalies both at  $T_m(B)$  and  $T_L(B)$ , both equal in magnitude, are well beyond the noise-level in the simulations. For the other parts of the  $C$ -curve, the uncertainties are of order the symbol size.

The fact that  $O_L = 1$  above  $T_L(B)$ , indicates that the long-wavelength vortex-line tension  $\varepsilon(T)$  vanishes. We may infer this from the change in  $O_L$ .

Furthermore, we have checked how  $T_L(B)$  varies with a change of aspect ratio  $L_x/L_z$  of the system. For  $f = 1/380$ ,  $\Gamma = 7$ , (not shown) we have considered systems of size  $L_x \times L_y \times L_z/\alpha$ , with  $L_x = L_y = L_z = 40, 80, 120$ , varying  $\alpha \in [1.00, 1.25, 1.50, 1.75, 2.00]$ . Within a vortex-line liquid picture, we should find  $T_L \propto \alpha^{19}$ . Instead, we find a change of less than 5% on increasing  $\alpha$  from 1 to 2, again difficult to explain within a vortex-line liquid picture of the molten phase above  $T_L(B)$ . This is supportive of a change in the connectivity of the vortex-tangle at  $T_L(B)$ , in a direction perpendicular to the magnetic field. In a vortex liquid with non-zero  $\varepsilon(T)$ , the vortex system is only connected across the system along the field direction.

The long-wavelength vortex-line tension may thus serve as a probe of the loss of order at the transition, playing the role of a generalized “stiffness”<sup>1</sup> characterizing the two vortex liquid phases above and below  $T_L(B)$ . More precisely, the two vortex-liquid regimes are characterized by breaking a  $U(1)$ -symmetry of the dual theory of the Ginzburg-Landau theory, on crossing the line  $T_L(B)$  from below.

We have obtained  $C$ ,  $\Upsilon_z$ ,  $S$ , and  $O_L$  for a wide range of filling fractions, see Fig. 1. The resulting  $(B, T)$ -phase diagram for the uniformly frustrated 3DXY model with the anisotropy parameter  $\Gamma = 7$  and  $B \parallel c$ , is shown in Fig. 1. In zero field, a 3DXY-transition separates the superconducting phase from the normal phase. In a finite magnetic field, we have three distinct phases: the AVL

for  $T < T_m(B)$ , the vortex liquid with line tension for  $T_m(B) < T < T_L(B)$ , and the vortex liquid without line tension for  $T > T_L(B)$ .  $T_L(B)$  is a critical line, the finite field counterpart of the zero field vortex loop blowout at  $T = T_c$ . In the low field regime,  $f < 1/600$ , the AVL melts directly into a vortex liquid with no line tension.

The dimensionless criterion determining the low-field regime of the melting line  $T_m(B)$ , is that  $f\Gamma^2 \ll 1^{20}$ . For our case, the merging of  $T_m(B)$  and  $T_L(B)$  occurs at  $f\Gamma^2 \approx 1/13$ , which is well within the low-field regime. Note that at more elevated fields,  $f\Gamma^2 > 1/4$ , the vortex lattice melting line is well described by both the XY-model and the 2D boson-analogy of the vortex-system, as recently nicely elaborated on by Koshelev and Nordborg<sup>20</sup>. However, from their Fig. 1, we note that deviations from universal properties of line-like melting of the vortex lattice starts to appear for  $f\Gamma^2 < 1/5$ , consistent with the above picture.

$T_m(B)$  meets  $T_L(B)$  at a tricritical point, see Fig. . The continuation of the melting line below the tricritical point is first order. We have observed a substantial increase in the  $\delta$ -function spike at the melting transition below the tricritical point, since the entropy in the transition at  $T_L(B)$  now contributes to a first order transition<sup>17</sup>. Note also that well above the tricritical point, the position of  $T_m(B)$  is adequately described by a Lindemann-criterion applied to the London-model including only field-induced vortex lines<sup>21</sup>. It is not clear, however, that such a model would give  $\Upsilon_z = 0$  in the entire molten phase.

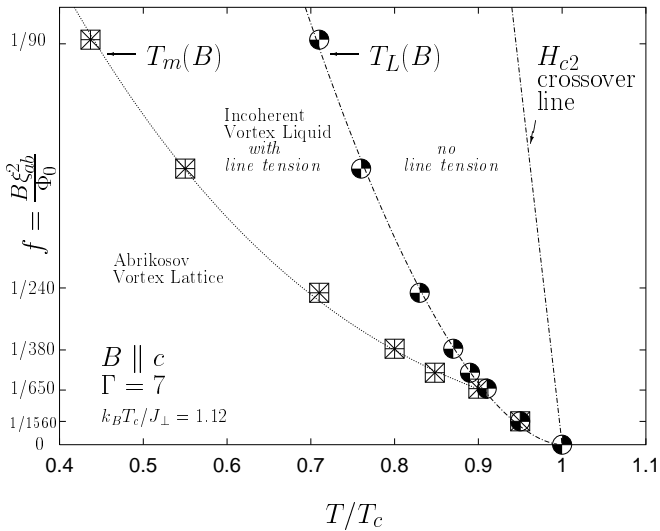


FIG. . The intrinsic  $(B, T)$ -phase diagram of an extreme type-II superconductor, obtained from the uniformly frustrated 3DXY model with  $\Gamma = 7$  and  $B \parallel c$ .  $k_B T_c / J_{\perp} = 1.12$ . The filling fractions  $f$  that are used are given by  $1/f = 90, 132, 290, 380, 506, 650, 1560$ . The lines are guides to the eye. The  $H_{c2}$ -line is found from the maximum value of the broadened peak of the specific heat in a finite magnetic field.

In summary, we have used large-scale Monte-Carlo simulations to analyze the characteristics of vortex-paths in a model of extreme type-II superconductors in the absence of disorder. An abrupt change in this characteristics reveals a phase-transition involving the breaking of a  $U(1)$ -symmetry, which is suggested to exist in zero as well as finite magnetic field. It is therefore distinct from the vortex lattice melting transition. This symmetry breaking is a consequence of a thermally driven vortex-loop “blowout”<sup>22</sup>. It results in a nonconserved number of thermally fluctuating connected vortex paths threading the entire system in any direction, including the direction perpendicular to a transverse magnetic field. *In other words, the connectivity of the vortex-tangle changes*<sup>13</sup>, and the insensitivity of  $T_L(B)$  strongly suggests that this is a feature that survives in the thermodynamic limit.

In principle it is also possible for a  $U(1)$ -symmetry breaking to be first-order, although in zero magnetic field this only happens for small values of  $\kappa$ <sup>23</sup>. In finite field this could change. More work is clearly needed to investigate in detail the universality class of the proposed transition at  $T_L(B)$ .

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